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HED Hydrodynamics in the Common Modeling Framework

OES ICF FY21 L2 Milestone #7429

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Within the Common Modeling Framework (CMF), the HED Hydrodynamics Project has implemented a common methodology, or "Authority", for modeling high energy density (HED) experiments by extending development of the Eulerian Applications Project code Authority, "EAPA," to include relevant physics models, customization tools and templates, and in situ and post-processing capabilities. Additionally, several models for small-scale HED experiments were successfully added to the CMF and simulations reproduce the results of preexisting, benchmarked input decks. We expect use of the CMF to improve our effectiveness in developing predictive capabilities for experiments ranging from small-scale planar single-interface, single-shock to multi-interface, multi-shock configurations and up through multi-shell inertial confinement fusion (ICF) implosions. Additionally, this will strengthen our ability to design future targeted experiments. Using the CMF infrastructure and Authorities for HED modeling has three key impacts. First, it enables a version-controlled, pedigreed and archived base model for each experiment with tools that allow easy setup, execution and analysis of simulations to assess and/or expose sensitivities to various parameters. Second, having a common base set of inputs and physics definitions helps identify systematic differences between models in the codes and experimental data to support code validation, and build confidence in our predictive capabilities. Finally, designed to work in concert with multiple programs and projects including PEM, IC, OES, V&V and DSW, the CMF supports improved collaboration and integration through shared model definitions, data, simulations and results, enhancing the workflow required to underwrite the knowledge base and capabilities ultimately required for stockpile stewardship.

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Introduction

Radiation hydrodynamics codes are built on many different physics models as well as input data such as equations of state and opacity. Due to the large number of input parameters, the solutions that match the data are often not unique. Code input settings can be configured in multiple ways, which complicate validation of physics models or comparisons across experiments and simulation models that have been developed by different designers. Over the past ten years, a new strategy has emerged to ensure standardization through the creation of a version-controlled common modeling methodology in which experiments are modeled with common settings defined by the modeling community's best practices. The Common Modeling Framework (CMF) is an infrastructure used to house common model methodologies, called “Authorities”, for different classes of problems. This strategy enables improved model validation through the use of large suites of experiments using common input parameters and physics settings.

The CMF is designed to work in concert with many programs, providing integration across Physics and Engineering Models (PEM), Institutional Computing (IC), the Office of Experimental Sciences (OES), Verification and Validation (V&V) and Directed Stockpile Work (DSW), leveraging the work of all CMF contributors. In addition to helping fulfill the goal of the ICF program to use experiments to advance our physics models, HED in the CMF will improve collaboration and integration with these other programs through shared model definitions, data, simulations and results. This will enhance the Data>Model>Validation>Application workflow required to underwrite the knowledge base and develop capabilities for the application of HED physics to stockpile stewardship.

A description of the ICF HED Hydrodynamics L2 milestone is given in Table 1. In brief, the goal of the milestone was to provide an initial implementation of HED experiments in the CMF through Authority and model development. The milestone is complete when simulations of the experiments are executed using a CMF Authority and results of the milestone are documented.

Table 1. ICF HED Hydrodynamics FY21 L2 milestone description.

Milestone (ID# 7429): Complete Initial Implementation of HED Authority in the CMF		
Level: 2	**Fiscal Year**: FY21	**DOE Area/Campaign**: ICF
Completion Date: June 30, 2021		
Subprogram: HED Hydrodynamics Project		
Participating Sites: LANL		
Participating Programs/Campaigns: OES ICF		
Description: The Common Modeling Framework (CMF) is designed to work in concert with many programs, providing integration across PEM, IC, OES, V&V and DSW, leveraging the work of all CMF contributors. In this milestone, the aim of the ICF HED Hydrodynamics Project is to provide an initial implementation of HED experiments in the CMF through authority and model development, creating a resource for all CMF users. In brief, advancement of the EAP authority will be accomplished through, • development and application of required physics packages needed for HED calculations, • CMF implementation of 1D and 2D HED experiment models, • development of quick-start HED templates for 1D and 2D models, and • an initial implementation of automated post-processing of HED simulation results.		

Completion Criteria: Completed when the simulations of HED hydrodynamics experiments are executed using CMF authorities and documented in a report.	
Customer: OES, ASC V&V, DSW	
Milestone Certification Method: A review by the ICF program manager is conducted. Professional documentation comprised of CMF authority development details, HED experiment model descriptions, and CMF model results is prepared as a record of milestone completion.	
Supporting Resources: OES ICF & C4, ASC CSSE	

Within the CMF, LANL has implemented a common methodology for modeling high energy density (HED) experiments in its Advanced Scientific Codes (ASC) project by extending development of the Eulerian Applications Project code authority, "EAPA." We expect this to improve our effectiveness in developing predictive capabilities for experiments ranging from small-scale planar single-interface, single-shock to multi-interface, multi-shock configurations and up through multi-shell ICF implosions. Additionally, this will strengthen our ability to design future targeted experiments. Using the CMF infrastructure and Authorities for HED modeling has three key impacts. First, it enables a version-controlled, pedigreed and archived base model for each experiment with tools that allow easy setup, execution and analysis of simulations to assess and/or expose sensitivities to various parameters. Second, having a common base set of inputs and physics definitions helps identify systematic differences between models in the codes, as well as in experimental data, to support code validation and build confidence in our predictive capabilities. Finally, designed to work in concert with multiple programs and projects including PEM, IC, OES, V&V and DSW, the CMF supports improved collaboration and integration through shared model definitions, data, simulations and results, enhancing the workflow required to underwrite the knowledge base and capabilities ultimately required for stockpile stewardship.

The final products of the milestone include:

1. CMF implementations of specific features and physics options required to incorporate HED models in the EAPA Authority, including
    a. Expansion of general functionality of the CMF and the EAPA Authority
    b. 1D and 2D laser package options
    c. Heat conduction options
    d. 3T plasma physics options
    e. Mix modeling options
    f. User control of EOS tables
    g. Freeze regions
    h. 1D primitives
2. Implementation of HED models into the CMF
    a. 1D and 2D ModCons with no laser
    b. 1D and 2D ModCons with laser package
    c. 1D and 2D MShock OMEGA models
    d. 2D Cylinders models in cylindrical-axisymmetric R-Z geometry and planar R-Theta geometry
3. Implementation of HED templates to expedite new experiment creation in EAPA
4. Implementation of in situ and post-processing tools for HED experiments
5. Customization examples
6. A step-by-step tutorial in Confluence on using the CMF
7. This report available on Confluence and as a white paper documenting the work performed for this milestone

Background

HED Hydrodynamics Project

One of the most significant challenges for the success of multi-shell targets is hydrodynamic stability. While all implosions are hydrodynamically unstable, multi-shell targets bring the additional challenges of multiple interfaces subjected to shock waves and capsule defects, such as the seams in the outer shells needed to insert inner shells. To evaluate the efficacy for double shell targets as a mix and burn platform, stability of the inner shells must be understood and control demonstrated. The project is broken into four key elements: hydrodynamics of the inner shell, defect hydrodynamics, turbulent mixing, and the common modeling framework. These elements, when combined, are expected to provide a comprehensive picture of not only the stability of the inner shell, but the stability and dynamics of each material interface for multi-shell implosions.

More specifically, the laser-driven experiments under the HED Hydrodynamics Project currently focus on benchmarking turbulent mix models. Mixing of materials at interfaces play a critical role in the performance of ICF implosions. LANL uses the BHR mix model [Besnard92, Stalsberg-Zarling11, Schwarzkopf14] in its simulations of both "hot spot" ICF capsules and in double shells. Thus, valid models for these integrated platforms require focused experiments to ensure confidence in our calculations. The projects here are aimed at examining multiple shocks across a layer, to which the double shell, inner shell or the dopant layers in a high gain hot spot capsule will be subjected. This project obtains data to validate various aspects of mixing in xRAGE [Gittings08] and FLAG [Burton92, Burton94], such as the BHR mix models, mix initialization models (primarily the new Modal Model [Rollin13]), multi-shock conditions, and convergence effects. Experimental results ultimately will be compared with turbulent mix models in HED/ICF regimes in conjunction with the ASC PEM and V&V programs. Together, all of this work supports our understanding of mixing to evaluate robust burning platforms for ICF. The results will provide confidence that BHR and the Modal Model can be applied to HED regimes found in ICF implosions and can be used for future designs.

The primary platforms under the project developed to achieve these goals are *ModCons*, *MShock* and *Cylinders*. For this milestone, models for each of these platforms, and the mechanics to apply the physics packages required to execute these models in xRAGE, were developed and implemented in the CMF. A brief discussion of the purpose for each of these platforms is given below. Further description of the platforms and their corresponding CMF models are described in the section on *HED Experiment Models and Results*.

The *ModCons* experiments on OMEGA-EP are designed to provide a data set for validation of the Modal Model, which has been implemented in xRAGE and FLAG for the initialization of the BHR mix model. The Modal Model informs BHR by evolving the initial perturbations on surfaces according to hydrodynamic instability theory until the flow has transitioned to fully turbulent. At this time, the BHR model is activated and initialized with values from the Modal Model. Validation of the Modal Model through the *ModCons* experimental platform will be achieved using measurements of the growth of multi-mode perturbations for Raleigh-Taylor (RT) and Richtmyer-Meshkov (RM) configurations from linear to highly non-linear regimes. The current principal goals of *ModCons* are to produce measurements of multi-mode perturbations for validation of the transitional Modal Model and to perform scaled-drive studies for the National Ignition Facility (NIF) *MShock* platform. These experiments extend our understanding of how initially laminar flows transition into turbulence, and will be used to help validate the implementation of the Modal Model in xRAGE. Recent improvements will allow us to fabricate, diagnose, and simulate multi-mode RM and RT experiments from the linear stage into the highly non-linear, and perhaps turbulent, regime with unprecedented fidelity.

The *MShock* platform is a multi-shock/multi-interface platform designed to examine Richtmyer-Meshkov hydrodynamic instability growth of perturbed layers due to both the interaction with multiple shocks from multiple directions, and the feed-through of perturbations from one side of the layer to the other due to instability growth and imprinting on those shocks. An ultimate goal for this platform is the capability to drive up to four shocks, two on either side of a thin foil, using the beams available at NIF. Near-term experiments will focus on evolution of a single-interface under two successive shocks from the same side for a variety of initial conditions relevant to our turbulent mix models. The current goals for *MShock* are to extract model parameters from the first-generation thin-layer data and compare to simulations, implement VISAR on a shock tube target for in situ drive characterization, and execute NIF *MShock* experiments (single-interface, two successive shocks) for several different interface perturbation initial conditions. The analysis work on the thin-layer data will establish a method for extracting a turbulence model parameter, which can be used, in addition to traditional metrics like mix widths, to provide more stringent constraints on our mix model performance for HED physics. This analysis method can then be extended to other HED data.

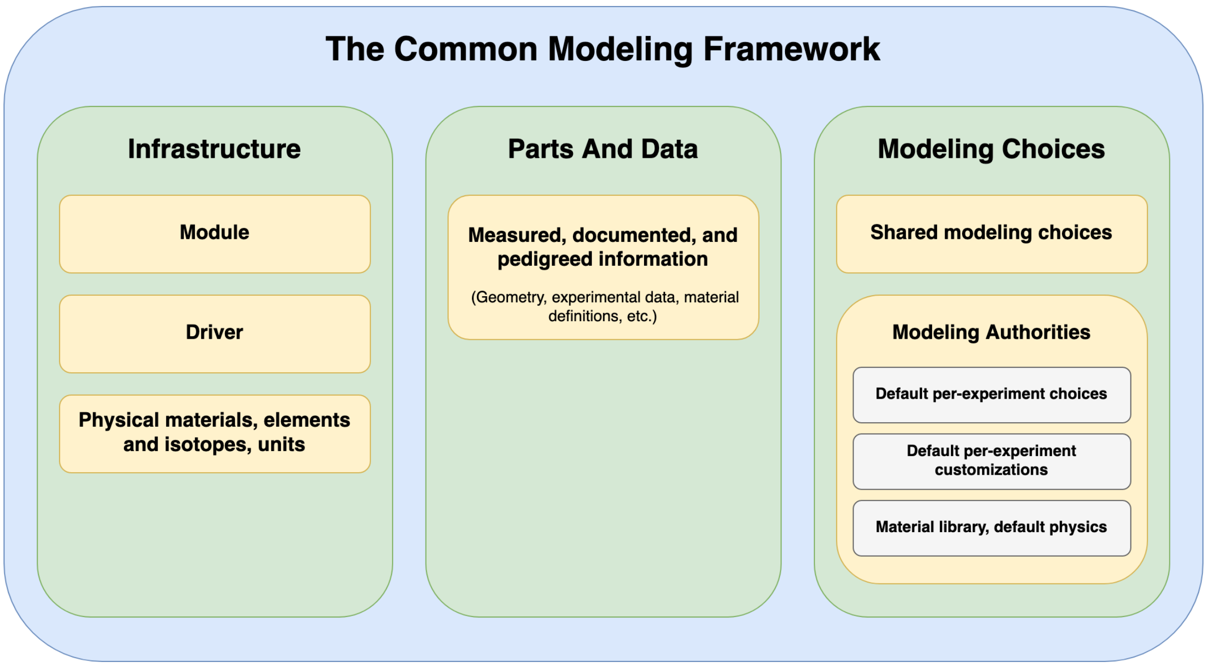
The *Cylinders* campaign provides an experimental platform to evaluate hydrodynamic instability growth in convergent geometries while preserving the ability to make high quality measurements. Convergent geometry is important because implosion brings in several effects that are not present in planar experiments, such as compression, Bell-Plesset, and differential effective Atwood numbers for bubbles and spikes. Initial experiments on the NIF have produced very high quality data at convergences up to ~5. Moving forward, the goal will be to achieve convergences of ~10, relevant for the inner shell of the double shell and large enough to validate the effects of convergence on our mix modeling. The platform may also provide a path to investigating the evolution of defects for implosions. The near term goals are focused on supporting double shell target development with an eye to investigating the instabilities currently using planar geometry for the case of ICF implosions. Current experiments focus on achieving higher convergences while designing a double cylinder target. The double shell design will enable studies of instabilities on the outer surface of the inner shell during implosions. Both of these efforts are central to quantifying uncertainty and improving predictive capability to enable a more quantitative assessment of double shells.

What is the CMF?

The Common Modeling Framework (CMF) is an extensive software project originally developed to provide an infrastructure to systematically develop, conduct simulations of, and evaluate experimental setups and modeling strategies for ALDX organizations and V&V projects. The CMF includes efforts across many program elements, from DSW-sponsored system baselines to ASC PEM-sponsored modeling parameters to ASC IC-sponsored modeling choices. Users of the CMF include primarily XTD and XCP scientists, but also staff from other divisions outside of ALDX. With a sophisticated repository to capture both current and historical work, the primary goal of the CMF project is to provide a single overarching structure to facilitate decision-making for the broader weapons program effort and to provide capabilities to a wide range of user communities. Over the last year and a half, development and utilization of the CMF has expanded to include programs under the Office of Experimental Sciences, in particular, the ICF HED Hydrodynamics Project for this L2 milestone, and C4's SAT project for development and validation of mix models.

The CMF is written in Python and consists of libraries and modules that grant users access to a wide range tools to store geometry, measured data for experiments, and modeling choices in a shareable format. Modeling choices can be user-defined or specified by an "Authority". Authorities, such as the Eulerian Applications Project Authority (EAPA) that is discussed in this report, are sets of default modeling choices that combine the data and decisions used to execute and post-process physics simulations. Authorities are typically code-specific and defined by a project, program, or group depending on the problems of interest. There are currently about a half dozen Authorities under development in the CMF that support each of the major physics codes: FLAG, Pagosa and xRAGE [Burton92, Burton94, Pagosa20, Gittings08].

Figure 1. Schematic of the CMF structure.



As seen in Figure 1, the CMF is generally organized into three main components: Infrastructure, Parts and Data, and Modeling Choices. The Infrastructure includes many under-the-hood utilities, such as the CMF module and the CMF driver, which provide a user-interface via command-line tools. This component also contains shared definitions and tools, including physical materials, elements and isotopes, and units. The Parts and Data directory is where all of the data that does not contain information that is considered user-choice or user-defined is stored. For example, Parts and Data contains measured information about an experiment, geometry, material composition and initial properties of a part (e.g., density, mass, temperature), agreed upon definitions of theoretical "experiments" or problems, information that is true regardless of what code or physics models you choose to simulate an experiment, data from experimental results, and pedigree of all of the above. Finally, user- or authority-defined per-experiment modeling decisions are located under Modeling Choices. These can include shared material models (e.g., equations of state, strength models, and burn parameters) and default physics choices that are automatically applied to any given experiment using a specified modeling Authority. Besides storing default parameters, an Authority may also contain experiment models with user-defined or per-experiment choices. For example, this may include specifying which conduction model to use, or identifying materials to include when modeling turbulence, or defining a mesh zoning strategy if it differs from the Authority defaults. Additionally, customization files that contain optional modeling decisions that may overwrite data or Authority defaults can be stored here.

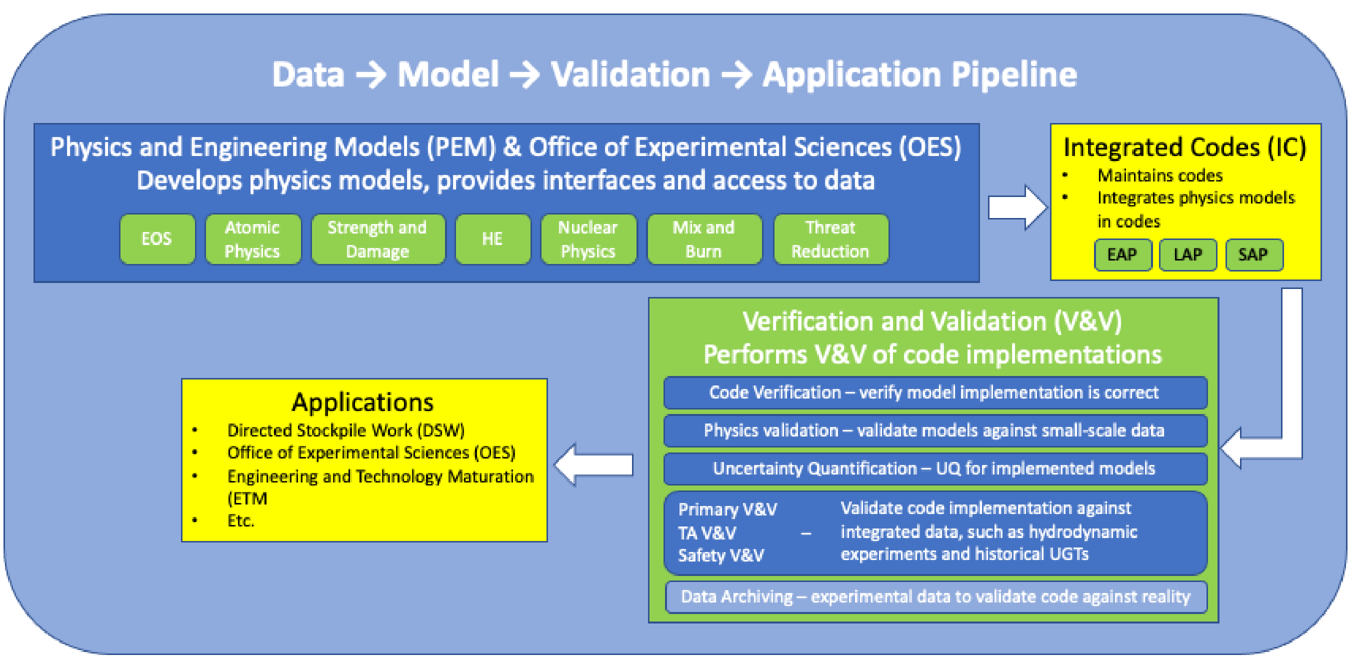
As discussed previously, the CMF is designed to work in concert with many programs and projects. Thus, we choose to utilize the CMF because it supports improved collaboration and integration among programs through shared model definitions, data, simulations and results, enhancing the workflow required to underwrite the knowledge base and capabilities ultimately required for stockpile stewardship.

There are many other advantages to working within the CMF. These include but are not limited to:

- Ability to leverage work of all CMF contributors: projects can share data and inherit models from each other, facilitating the flow of information from small-scale to integrated experiments (see Figure 2)
    - Reduced start-up time that is usually required with initial development of experiment models
    - Sharing of data and models better utilizing time and resources allowing modelers/users to focus on physics
- Improved modeling fidelity
    - Pedigree creates confidence: modelers include sources/references for data and modeling choices, taking the mystery out of model parameters, data and other options
    - Archiving leads to efficiency: data and models are reliably stored rather than at risk of being lost, eliminating the need for staff members to endlessly "reinvent the wheel"
    - Version control: models can be continuously improved and updated without losing original versions, i.e., changes can be tracked
- Standardization of file formats improves readability and reduces errors
- Use of Python, a common coding language: a highly accessible programming language, readable and maintainable, compatible with major platforms and systems
- Cross-code comparisons: creates the potential to share models across multiple Authorities and codes

A major advantage mentioned above is the workflow pipeline which enables integration and collaboration between projects, from the experimentalists that provide the data to the scientists who develop, execute and validate models, which subsequently are applied to the primary applications of interest. The ICF HED program contributes to all portions of the pipeline, providing small-scale data for model development and validation (mix and burn, lasers, etc.), informing V&V decisions, and ultimately incorporating the results into modeling choices for large-scale applications that contain integrated data.

Figure 2. CMF as a workflow pipeline, adapted from [Hickmann21].



Code Development, Models and Results

EAPA development

The Eulerian Applications Project Authority (EAPA) is a CMF modeling authority that is responsible for setting up and running physics simulations with the xRAGE code. Prior to the work accomplished in this milestone, the development of EAPA was essentially stalled due to a lack of options for any specific class of problems as well as a shortage of CMF code developers. We chose to implement new functionality that incorporates HED hydrodynamics experiments into EAPA, as opposed to creating a new modeling authority from scratch, for a variety of reasons. First, the HED experiment simulations are executed in xRAGE, and the basic infrastructure was already in place to store models and create input decks for this code. Instead of reinventing the wheel, we expanded on what was already developed. Second, when LANL transitioned to a work-from-home schedule due to the COVID-19 pandemic, more code developers became available to work on general support for this authority, allowing us to focus on adding physics package options rather than on general infrastructure development. Shared development on this authority led to more support for general functionality, which contributed to a more robust infrastructure for storing and improving our physics models. Lastly, in improving EAPA for HED modeling, we improved the authority as a whole, providing an example for future development.

In order to incorporate the HED experiments into EAPA, a list of specific features and physics options had to be developed in the authority, such as HED-specific physics options, HED experiment-specific templates, post-processing tools, tutorials, and documentation. These features are discussed below.

Physics Packages

Using Python code design, we were able to leverage Python modules to re-design EAPA's physics package library so that any given physics option can be imported individually, as needed into a *perExperiment* file, analogous to the way that the packages are turned on and off in xRAGE. Specific physics options that were added are:

- Freeze regions
    - A freeze region is a geometric region in the hydro mesh inside of which the material state is reset to its initial values after each time step. For the purpose of these simulations, freeze regions enable the user to force shock jump conditions at a boundary, producing a steady shock. This is an excellent method of low computational cost and physics complexity to model experiments where such a shock description is valid. One example where this can be leveraged is *ModCons*, where due to the duration of the laser pulse, the entire linear phase of the instability growth occurs under these conditions.
- Laser package, 1D and 2D
    - The laser package is a model developed by the Laboratory for Laser Energetics for use in the DRACO code [Igumenshchev09], which has since been borrowed and adapted for xRAGE. The model performs a cylindrically-symmetric 3D ray trace of the laser beam based on user-specified input, on its own mesh, and then transfers the result to a 2D xRAGE hydro mesh, modeling the energy deposition via inverse Bremsstrahlung absorption. The laser package also includes a simpler sector ray trace for 1D calculations, for which the full ray trace is not necessary.
- 1D primitives
    - Regions or parts can be defined through internal primitives that include simple regions, perturbed boundary regions, mask regions, overlay regions and imported regions.
- Mix and mix initialization
    - *Mix model options: BHR-2, BHR-3-1 (default), BHR4*. The BHR model is a multi-species turbulence model developed to address the physics of multi-material compressible turbulent

flows in miscible fluids. It provides a complete closure for the filtered variable-density Navier-Stokes equations, along with appropriate modeled turbulent transport equations. BHR assumes a fully turbulent flow.

  - *Mix initialization model options: fixed S0-K0 (default), Modal Models 1* and *1e, Modal Models 2* and *2e, Tracer BHR* [Rollin13, Braun20]. These models provide turbulence model variables used to initialize the BHR turbulence model. Setting a default turbulent length scale (S_0) and turbulent kinetic energy (K_0) at the time the BHR physics package is activated is the current default method for initialization. The Modal Model is a different strategy that generates profiles of turbulent model variables to initialize the BHR model when specific criteria are met, e.g., critical turbulent Reynolds number = 2500, and the mix model is activated. Tracer BHR is used to extend the Modal Model approach into turbulent regimes "when the mixing layer width predicted by the Modal Model is smaller than the local mesh spacing" [Crestone08] but the Modal Model has met the criteria to transition to BHR. It allows the mixing layer to continue to evolve until the layer is larger than the local grid spacing.
  - Examples of how to use the mix and mix initialization classes available to EAPA can be found here: Mix in the CMF.
- User control of EOS tables
  - Formerly, if an EOS table was used in an experiment, the variables were hard-coded into the CMF infrastructure. This restricted any user control. This update gives the user the option to specify values for a given variable in an EOS table that is written into the TEOS file at run-time.
- Heat conduction
  - xRAGE includes support for various conductivity models, including tabular SESAME conductivity, Spitzer conductivity, and a couple of simpler analytic models. At present, we have included CMF support for Spitzer conductivity, which is the most relevant model for laser-driven HED experiments.
- 3T
  - A three-temperature description (electron, ion, and radiation temperatures) in conjunction with isotopics is required to model the laser deposition as well as the separate electron and ion heat conduction in the ionized plasmas that develop in these experiments.

HED Templates

Because the task of creating files and their links in the CMF can be tedious and confusing to the user, we chose to implement 1D and 2D templates that complete this task automatically. Furthermore, the template provides common HED physics options and provides a narrative of what each section in the *PartsAndData* and *perExperiment* files accomplish, creating a more user-friendly and less error-prone experiment creation experience to the user.

In Situ and Post-Processing Tools

The task of providing general post-processing tools for a given experiment is monumental. As a proof-of-concept for this milestone, we chose to narrow the task to provide some HED specific post-processing tools that are commonly used for the experiments we included here. We hope that the framework provided can be expanded and supply a convenient way for users to add their own post-processing tools to be used in the CMF.

Below, we present an introduction to *RageView* and results from its application to a CMF EAPA *ModCons* simulation. Additionally, in-situ and post-processing using workflows developed with *Fusion* [Biwer21] are dicussed. In this case, these tools have been applied to analysis of a CMF EAPA *Cylinders* calculation.

RageView Post-Processing Tools

The *RageView* post-processing tools add the capability to explore xRAGE simulation data through the plotting of HDF5 and tracer data. *RageView* is available to use with a command-line interface when the CMF module is loaded. In addition, *RageView* is a Python module, so classes and functions that are used to store, label, scale, and plot data can be imported into one-off scripts or implemented in CMF-specific routines, such as EAPA's "post" routine.

RageView as a suite of command-line tools:

Using the command-line interface, one can use *RageView* to view one- and two-dimensional HDF5 data as well as tracer data from an xRAGE simulation. Data visualization is accomplished through the use of Python plotting tools that provide a minimalist GUI so that the user can explore simulation data with a lightweight and easy-to-use program. Once the CMF module is loaded, one can view the documentation for *RageView* through the command-line help message: "rageview -h". From here, the available tools are:

```
rageview watch [options] <run> <var>
```

"watch", which allows the user to visualize one-dimensional HDF5 data by showing two plots: the first shows the variable as it evolves in time and the second shows a line profile of that variable at a given time-step. An animation can be played or the time-step can be advanced using the arrow keys. A specific time-step can be chosen by clicking on the first plot;

```
rageview show [options] <run> <var> [<var2>]
```

"show", which allows the user to visualize one- and two-dimensional HDF5 data by playing an animation of the variable as it evolves in time. The user can play the animation, or step through with the arrow keys. In addition, the user can click on the plot or pass in a flag to view a line profile at a given location;

```
rageview plot1D [options] <run> [<var>]
```

"plot1D", which allows the user to plot the one-dimensional HDF5 data;

```
 rageview plot_tracers [options] <run> <var>
```

and "plot_tracers", which allows the user to plot tracer particle data versus time. If there are multiple tracers in a run, the user can specify which tracer to plot by providing the tracer number.

As seen above, each tool must be provided with a run directory and the variable(s) that the user wishes to view. The options provide further capability and vary from tool-to-tool. See Figures 3 and 4 below for examples of each tool in action.

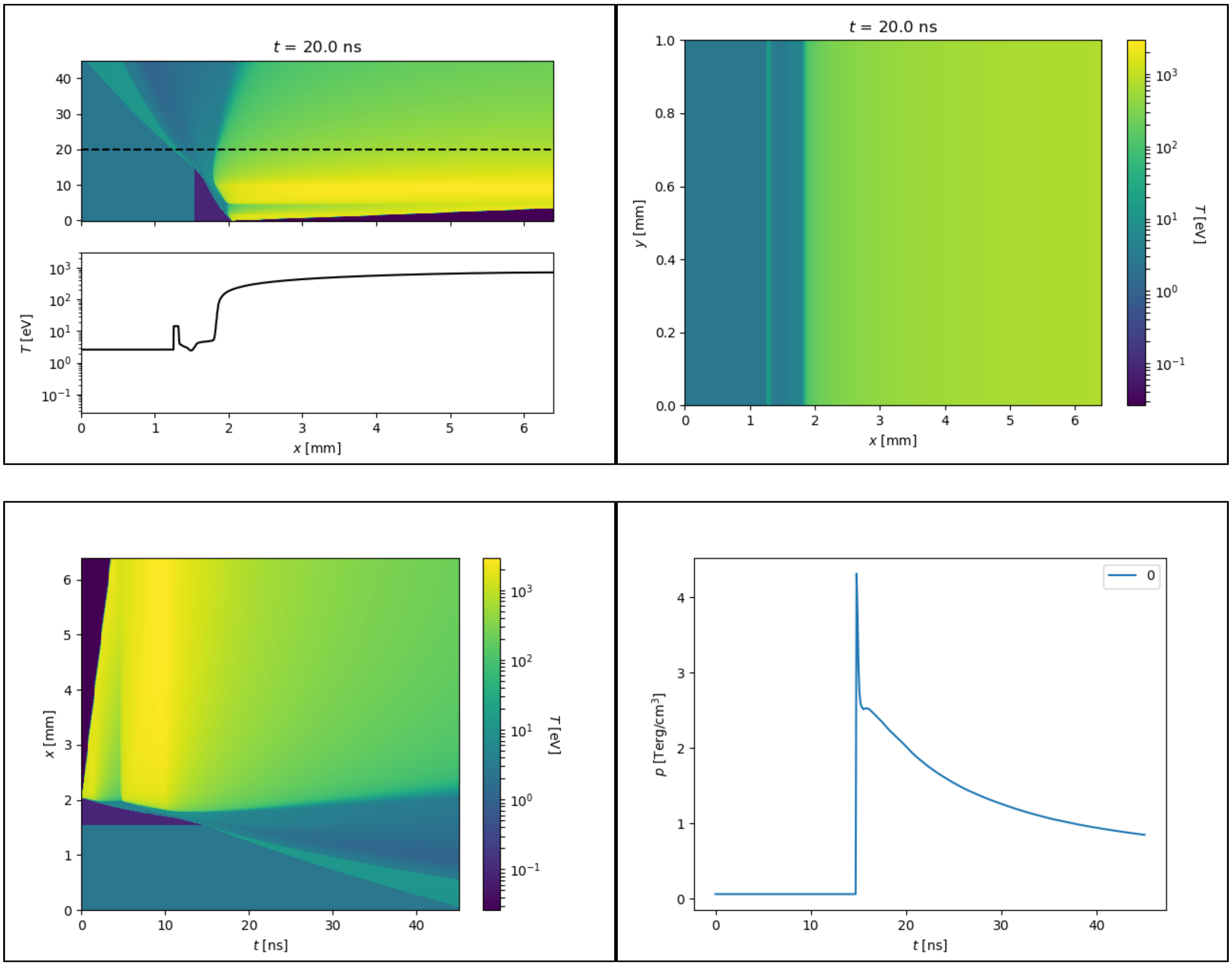


Figure 3. Plots produced using the *rageview* command-line interface to explore HDF5 and tracer data from the *ModCons* 1D experiment. Clockwise starting with upper left image, these plots were produced with the following *RageView* tools: watch, show, plot_tracers, plot1D.

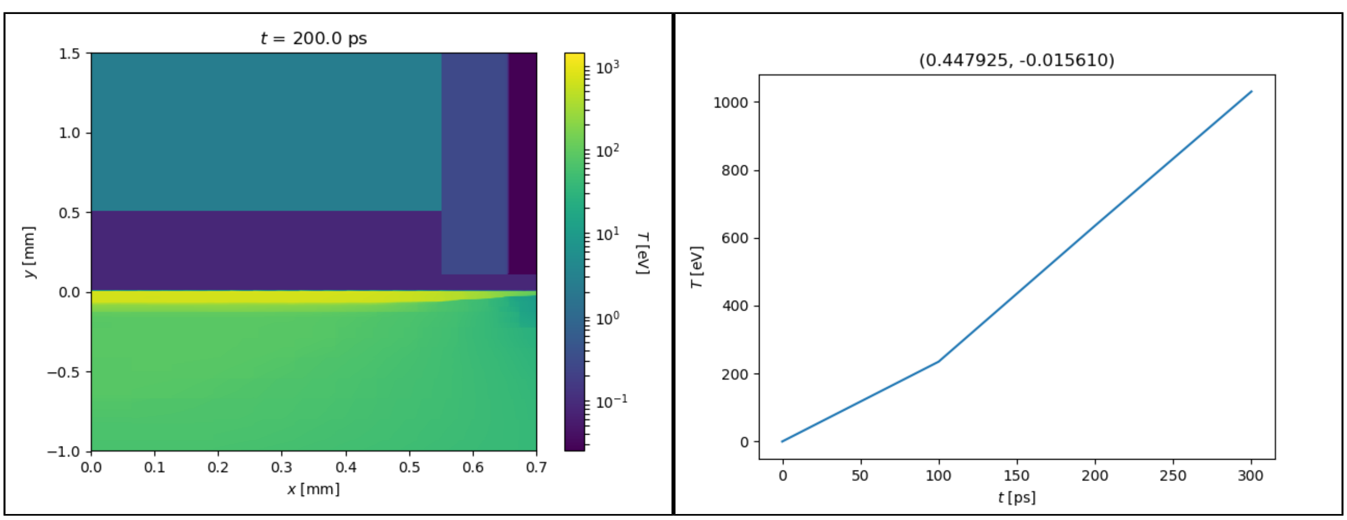


Figure 4. Plots produced using the *rageview show* tool to explore HDF5 data from the *ModCons* 2D experiment. The first plot shows the temperature at an early time-step and the second shows a line profile near the ablation surface that was extracted by clicking on the first plot.

RageView as a Python module:

Because *RageView* is written as a Python module, its classes and functions can be imported and used in other post-processing routines. Particularly useful are classes that can be used to store, label, scale, and plot HDF5 and tracer data. For this milestone, we used *RageView* to implement a post-processing routine in EAPA as well as a script to compare experimental data to CMF-generated simulation data for the one-dimensional OMEGA-EP *ModCons* experiment (see Figure 5).

```
from cmf.pref.eapa.posttools.rageview import RageView
```

EAPA's "post" routine currently produces a directory called "post" in which tracer data, if present in the run, for each variable is plotted versus time and saved as PDF files in a sub-directory called "tracer_plots". This is primarily a proof-of-concept routine and in future work will be extended to include more automated post-processing results.

```
cmf post <auth> <experiment>
cmf post eapa modcons_1d
```

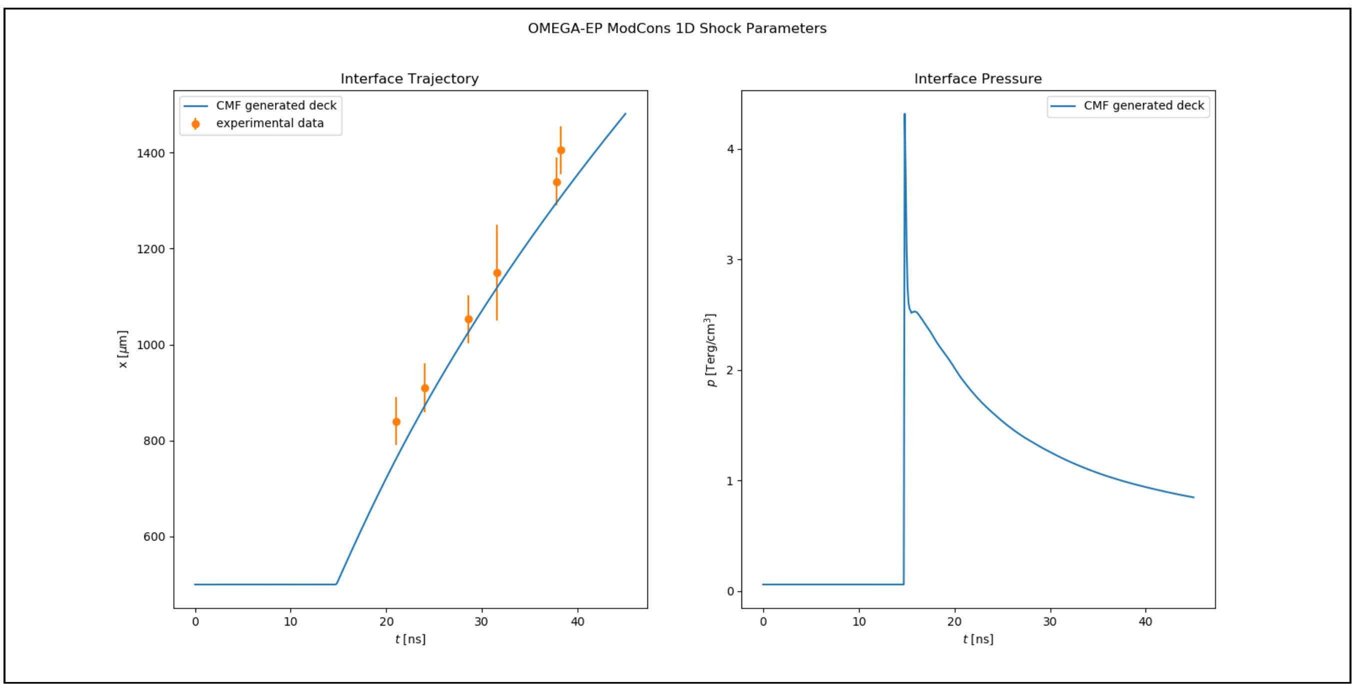


Figure 5. One-off plot utilizing the *RageView* module to store and plot tracer data.

Future work in *RageView* includes:

- increasing robustness of command-line tools with better error catching and warning messages,
- extending EAPA 'post' routines to write more automated post-processing data, perhaps allowing specific routines to be called by a specific experiment, and
- improving documentation in the *RageView* module and providing examples of its use in Python scripting.

In Situ- and Post-Processing with Fusion

Reliable automation of analyses is indispensable for increasing productivity, and essential for continuous integration or executing large workflows, e.g. for 3D *Cylinders*, over many time-steps or numerous datasets from parametric studies. Two approaches to automate a workflow are shown in Figure 6, either: in situ, i.e., perform the analysis while the simulation is running and has data structures in memory, or in post-processing after the simulations have written the mesh, particles, and boundaries to data files. We have developed workflows within *Fusion* [Biwer21], which is a library of workflows that can be called in situ or in post-processing. These workflows merge parallelized calculations and image renderings with visualization applications. *Fusion* is built on top of the CMF software stack and, therefore, can be called independently or within CMF customizations. As of 2021, current releases of xRAGE are now built with *ParaView* and once the EAPA Authority advances its default xRAGE version, these workflows can be incorporated directly into the CMF. Here, we report three advances: development to enable the *ParaView* in situ adaptor in EAPA (e.g., write images of the mesh), a robust data exploration workflow applied to EOS studies for *Cylinder* experiments, and a workflow management system that has been integrated into open-source software.

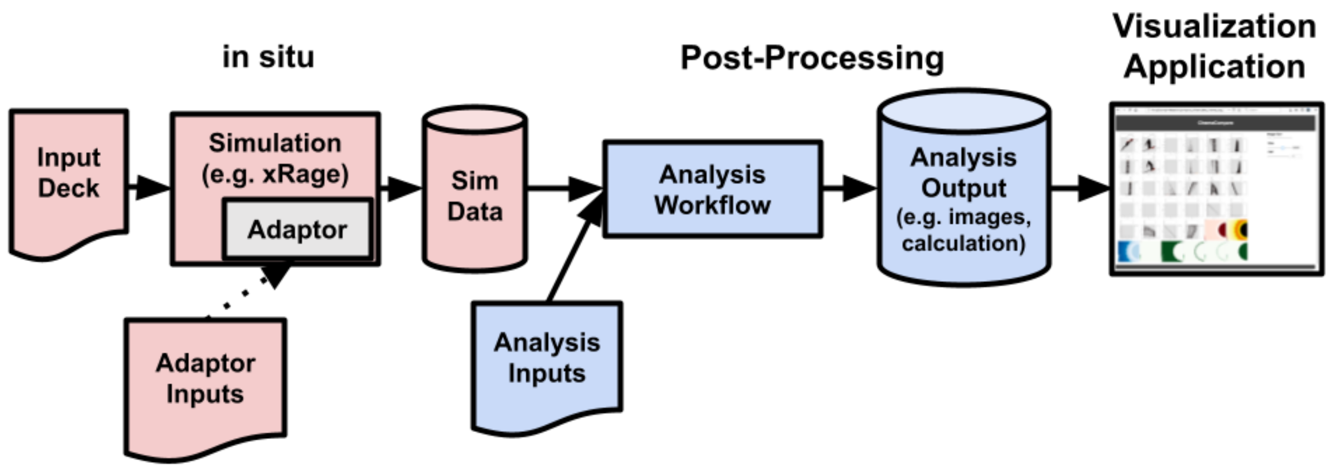


Figure 6. Workflows can be run either in situ (red) using the adaptor (gray) inside the simulation where calculations are executed or files are written while the simulation is running, or in post-processing (blue) using data files the simulation writes. For either in situ or post-processing, workflows can be designed to work with visualization applications, such as the *Cinema* viewer for image databases [Ahrens14] shown on the right.

The workflows we have developed leverages *ParaView* [Ahrens05] and the *ParaView* in situ adaptor [Ayachit15, Patchett17], which has been added into ASC integrated codes such as xRAGE, FLAG, and Pagosa, as well as other LANL-developed codes such as FleCSALEMM [Daniels20]. The in situ adaptor has most prominently been used to reduce the I/O strain of data files on filesystems [Biwer19]; however, it is capable of scripting all the mesh, particle, and geometric operations, e.g., data selection and parallelized calculations, and visualizations that *ParaView* can perform. There are two key benefits to this approach. First, *ParaView*'s algorithms are implemented at scale and handle the difficulties of parallelization underneath a simple Python API for the user designing the workflow. This lowers the learning curve for new users designing their own workflows from a library of documented examples. Second, our workflows can be readily applied across the LANL codes that have implemented the *ParaView* in situ adaptor.

Using this framework in the context of HED, we developed a data exploration workflow used to investigate the robustness of EOS modeling choices for OMEGA *Cylinder* experiments using xRAGE [Palaniyappan20, Sauppe20A, Sauppe20B]. The workflow produces a *Cinema* [Ahrens14] image database that can be viewed using a web browser as shown in Figure 7. The workflow allows the user to sample a material and plot the data selection on the mesh as shown in Figure 7a, produce a 2D histogram of variables with marginalized 1D distributions as shown in Figures 7b-c, and view images of the mesh as shown in Figures 7d-f. If the user plots EOS variables, e.g., pressure versus temperature that are written to the tabulated EOS file, then the 2D histogram can be overlaid on top of the EOS table. This workflow is not specific to OMEGA *Cylinder* experiments or xRAGE and it can be used for other simulations using the *ParaView* in situ adaptor. Although, we present this data exploration workflow for a post-processing use case to compare two simulations, the images can be produced in situ while the simulation is running. For example, the user could write images of the variables on the mesh while the simulation is in progress, as depicted in Figure 6 in which "Sim Data" is an image file. In addition, to plot samples on top of the EOS table, we were interested in producing a workflow for extracting the shock position over time as shown in Figure 8. This workflow has an option to extract a line profile through the mesh to produce overlay plots like the one in Figure 9.

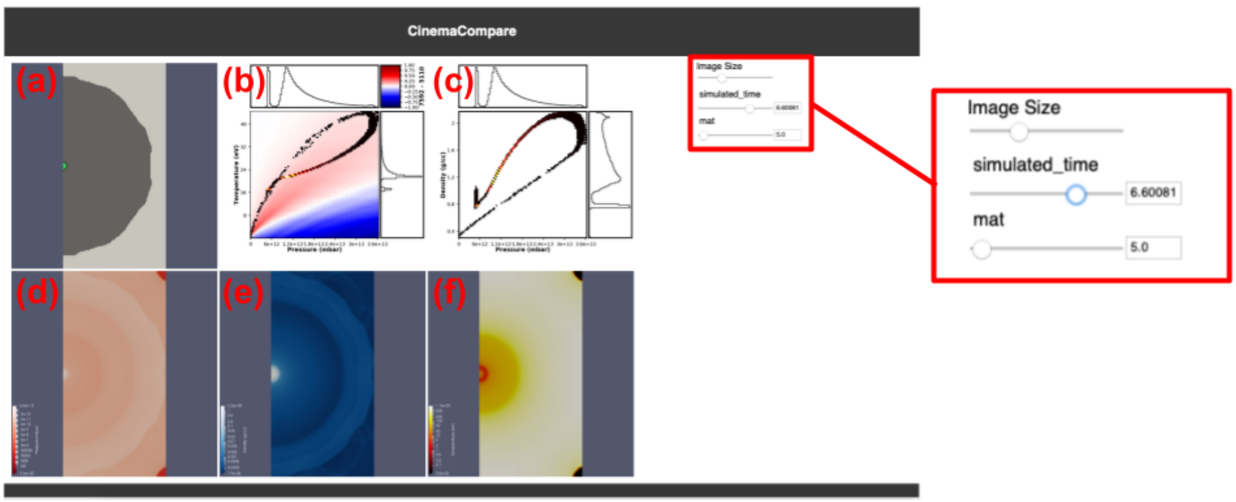


Figure 7. The output of the data exploration workflow is an image database rendered in a web browser which allows the user to scroll through variables such as time or material ID as shown in the red excerpt. The workflow samples a material and images are: (a) the region of the mesh of the material of interest is highlighted in neon green, (b) and (c) contain 2D histograms sampled from the material of interest, and (d), (e), and (f) contain plots of variables (e.g., pressure, density, and temperature) on the mesh.

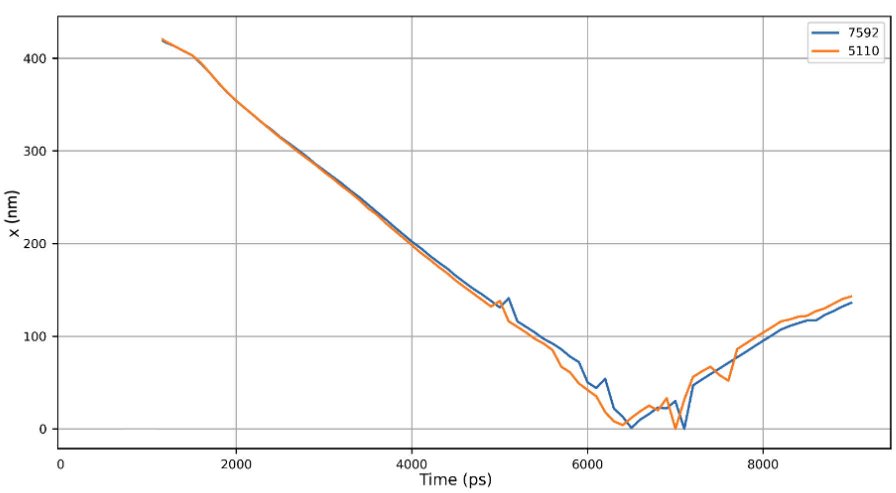


Figure 8. Line profiles extracted from two OMEGA *Cylinders* simulation. The simulation using SESAME 7592 EOS (blue) has a slower shock, noticeable beginning around 4000 ps, than the simulation using LEOS 5110 EOS (orange).

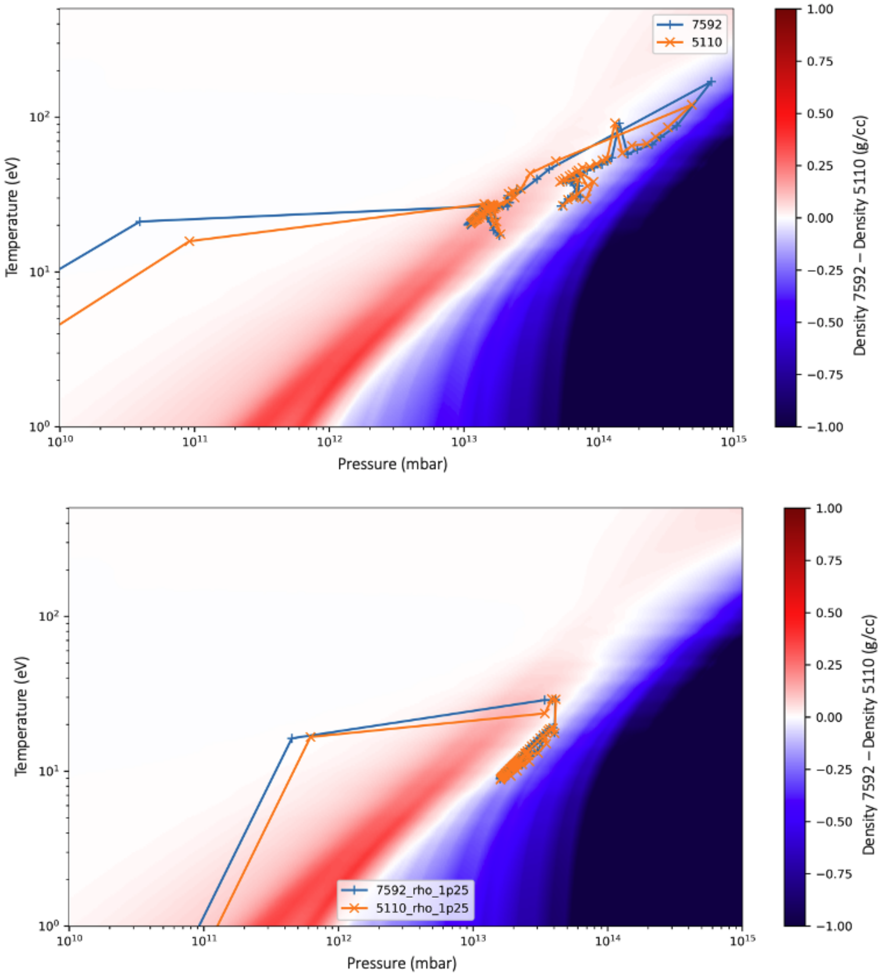


Figure 9: The shock temperature and pressure overlaid on the difference of the SESAME 7592 to LEOS 5110 tabulated EOS table. Red regions correspond to SESAME 7592 returning a higher density, blue regions correspond to LEOS 5110 returning a higher density, and white regions corresponds to regions where the two tabulated EOS tables return similar densities. Left: Using an initial CH foam density of 0.3 g/cc. Right: Using an initial CH foam density of 1.25 g/cc.

As a use case for this data exploration workflow, we compare simulations varying EOS modeling choices for OMEGA *Cylinder* experiments. For example, using the LEOS 5110 EOS, instead of the SESAME 7592 EOS for CH (polystyrene), produces faster shocks as shown in Figure 8. Although the difference in shock position in Figure 8 is consistent within the level of precision of experimental data, we use this data exploration workflow to determine the cause. Figure 9 shows a version of the 2D histograms from the workflow in Figure 7 used to compare two simulations. The shock pressure and temperature over time is overlaid on the difference of the SESAME 7592 and LEOS 5110 EOS. A red region corresponds to a region where SESAME 7592 returns a higher density and a blue region corresponds to a region where LEOS 5110 returns a higher density. For a region of initial densities between 0.1 g/cc and 0.9 g/cc, we observe this small difference in shock positions in Figure 8, which corresponds to the shock entering the region where SESAME 7592 returns a higher density, slowing the shock. Outside of this region where the shock speeds are comparable between the LEOS 5110 EOS and SESAME 7592 EOS, the two shocks predominantly stay in the white regions, where the two EOS return similar results, and an example at 1.25 g/cc is shown in Figure 9. This workflow was used to compare several other EOS modeling choices such as using other CH EOS (SESAME 7591 and 7592, and LEOS 5110 and 5105) and Al marker EOS (SESAME 3719 and 3720, and LEOS 130), which produced similar consistent results. In addition, we use this workflow to observe how varying the resolution of the tabulated EOS that xRAGE produces, i.e., changing the number of isobars, isotherms, and limits of the table, affects the results to verify the tabulated EOS was not sensitive to small changes in resolution.

Creating a large image database can be a computationally expensive operation. For example in Figure 7, a user investigating the change in initial density on shock position may extract samples of the simulation mesh over the number of mesh variables, V, number of materials, M, and number of time-steps, T, which will scale as V x M x T; for even five variables, five materials, and fifty time-steps the user will sample the mesh 1250 times. In order to accommodate large workflows, we developed a workflow management system to curate large submissions to distributed-computing clusters' queues which has been integrated into open-source, LANL-developed projects such as *Foresight* [Grosset20]. However, due to potentially large image databases we provide an alternative, where the user can write a *ParaView* state file instead of an image database, and explore the results dynamically in the *ParaView* GUI as shown in Figure 10. The state file will set up the GUI to plot the mesh, extract samples and overlay them on the EOS table, and plot the selected data over time.

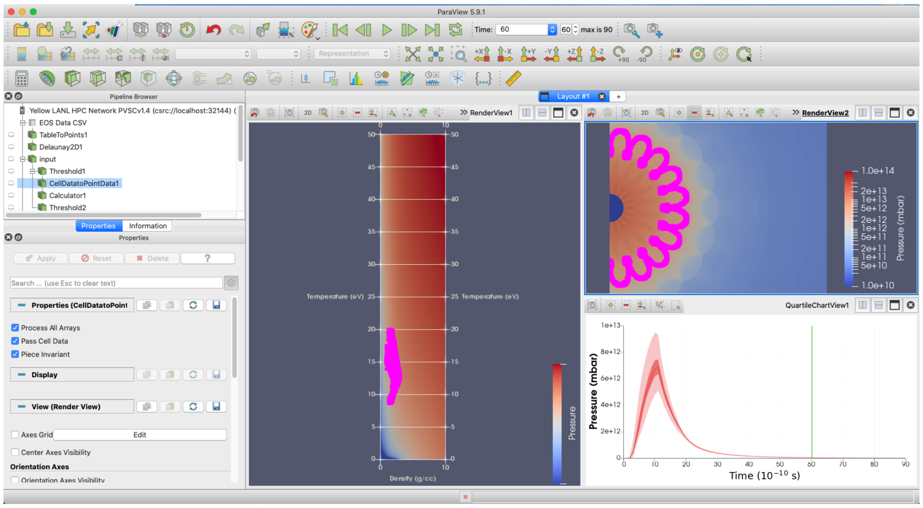


Figure 10. The data exploration workflow producing a *ParaView* state file to interact in the GUI as an alternative to an image database.

Tutorials and Documentation

In order to guide users through the process of adding, setting up, and running an experiment with EAPA, we provided a step-by-step tutorial on Confluence.

A tutorial on running the post-processing data exploration workflow in Figure 7 is provided here.

CMF and Authority Development Results

The results of our work for this milestone allow a user to set-up and run existing HED experiments or check-in a new experiment utilizing our HED templates. Most of this work is accomplished through the use of command-line tools that are available on HPC machines through the CMF module. To demonstrate the results of our work, we walk through the process of adding, customizing, running, and analyzing an HED experiment with the CMF below:

1. Make sure you are using the right CMF version and load the CMF module
2. Start from HED template

   ```
   createNewExperiment <auth> <expName> <expType>
   createNewExperiment eapa myOneDHEDExp oneD_HED
   createNewExperiment eapa myTwoDHEDExp twoD_HED
   ```

   a. See "Creating an experiment from a template" for more details
3. Edit the perExperiment and PartsAndData files utilizing HED physics packages
4. Set up and run experiment(s)

   ```
   cmf setup <auth> <expName> --subdir
   cmf setup eapa modcons_1d --subdir

   cmf setup-run <auth> <expName> --subdir
   cmf run <auth> <expName>
   ```

   a. See "Basic CMF commands" for more details
5. Apply a customization (optional)

   ```
   cmf setup <auth> <expName> --authCust
   ```

   a. See "Customizing the experiment" for more details
6. Run post-processing tools (optional)

   ```
   cmf post <auth> <expName>
   cmf post eapa modcons_1d
   ```

   ```
   rageview watch <run_dir> <var>
   rageview watch . tev
   ```

7. Documentation/Resources:
   a. How to add an experiment to EAPA
   b. Basic CMF commands
   c. How to build and/or view CMF documentation
   d. CMF Releases

HED Experiment Models and CMF Results

Below, we will describe several experiments for which simulations rely on the previously-discussed physics packages we have implemented in the CMF. A common feature of these experiments is that they usually involve some kind of ablator material (often plastic) which is either directly driven by illuminating the ablator itself with laser light, or indirectly driven by illuminating a cylindrical gold hohlraum, which absorbs laser energy and in turn re-radiates it towards the ablator in the form of X-rays. The experiments we include are all directly driven; a dominant process in indirect drive is radiation transport, which we are still working on implementing in the CMF. We hope to include some indirectly-driven examples in the near future.

Typically, a second material of differing density is placed against the ablator creating a density gradient, and one or both of the materials can be machined with a perturbation at their interface. In direct drive, the laser creates a high-temperature, high-pressure ablation plasma which drives a shock into the system resulting in hydrodynamic instability at the interface. In order to model this process, a simulation fundamentally must include a hydrodynamics model and some method of driving the system. Possible drive methods are an energy source or a freeze region (essentially forcing shock jump conditions at a boundary), both of which are now implemented in the CMF, or a laser model. A major focus of our recent work has been implementing support for the laser model in xRAGE, which was taken from the DRACO code and included in xRAGE by LANL's XCP staff. The laser model requires a number of settings in order to set up the configuration of the laser beams, and additionally requires that a simulation include 3T physics, isotopics, and heat conduction. The first two of these are required for modeling the deposition of laser energy into the system, while heat conduction is the dominant mechanism by which energy is transported from the laser deposition region to the shock front.

Modcons, 1D & 2D

The *ModCons* campaign is a series of directly-driven, planar instability experiments performed at the OMEGA-EP facility. The experiment consists of a solid plastic ablator placed against a piece of lower-density foamed plastic. An image of a typical experimental system is shown in Figure 11.

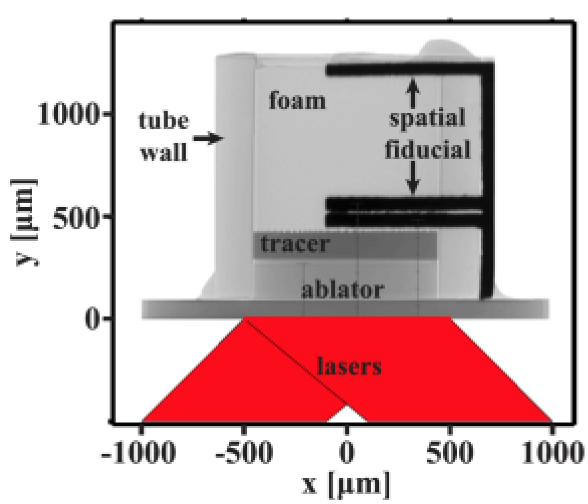


Figure 11. A pre-experiment radiograph of a *ModCons* target, showing relevant parts of the system.

The ablator includes a tracer layer doped with high-Z iodine in order to improve contrast for the radiography diagnostic. The unstable interface is between the tracer and the foam and, in the figure, the multi-mode seed perturbation is visible at this interface. The laser irradiates the system from the bottom, driving a planar shock upwards.

In addition to the hydrodynamics physics package, an xRAGE simulation of this experiment requires the laser model and the 3T, isotopics, and heat conduction packages as described above. Figure 12 shows the evolution of various parameters as predicted by the CMF-generated input deck (black and gray curves) as compared to our existing, benchmarked input deck (red and pink curves) and experimental data (open circles).

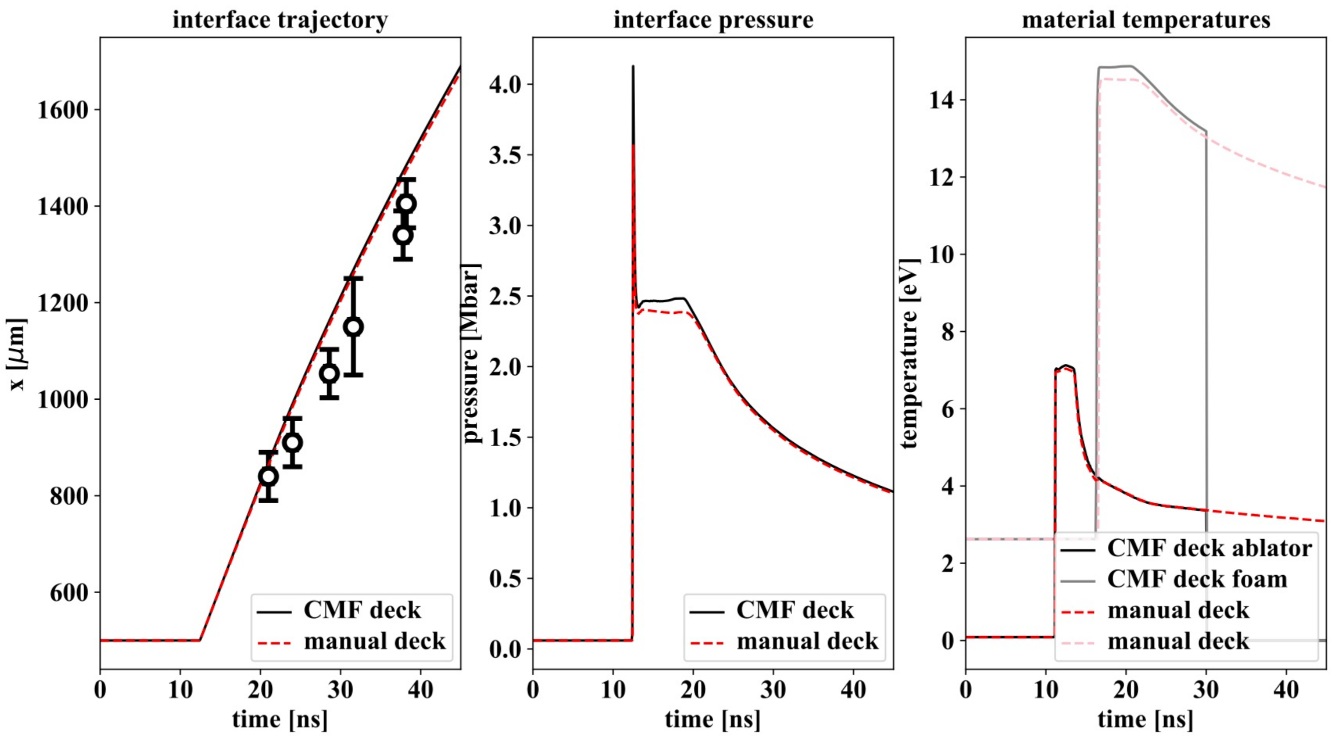


Figure 12. Various shock parameters as predicted by a 1D CMF-generated deck modeling the OMEGA-EP *ModCons* experiment. From left, plotted are the trajectory of the shocked simulation, the pressure at the shocked interface, and the temperatures of the two materials near the interface.

These parameters are all properties of the material interface; from left, plotted are the trajectory of the shocked interface, the pressure at the interface, and the temperatures of the two materials near the interface. From the figure, we see that the CMF-generated deck exhibits nearly-identical behavior to our benchmarked deck, and compares well to experimental data.

We also performed the same simulation in 2D, again using a CMF-generated deck. The physics in this simulation is substantially similar to the 1D version, except the laser model is now able to perform a fully-3D ray trace of the laser beams at every time-step. This allows the simulation to account for the full geometry of the laser setup, including each separate beam with its own angle of incidence, as well as a more detailed description of possible energy losses due to photon scattering in the ablation plasma. The shock and interface behavior from this simulation are shown in Figure 13.

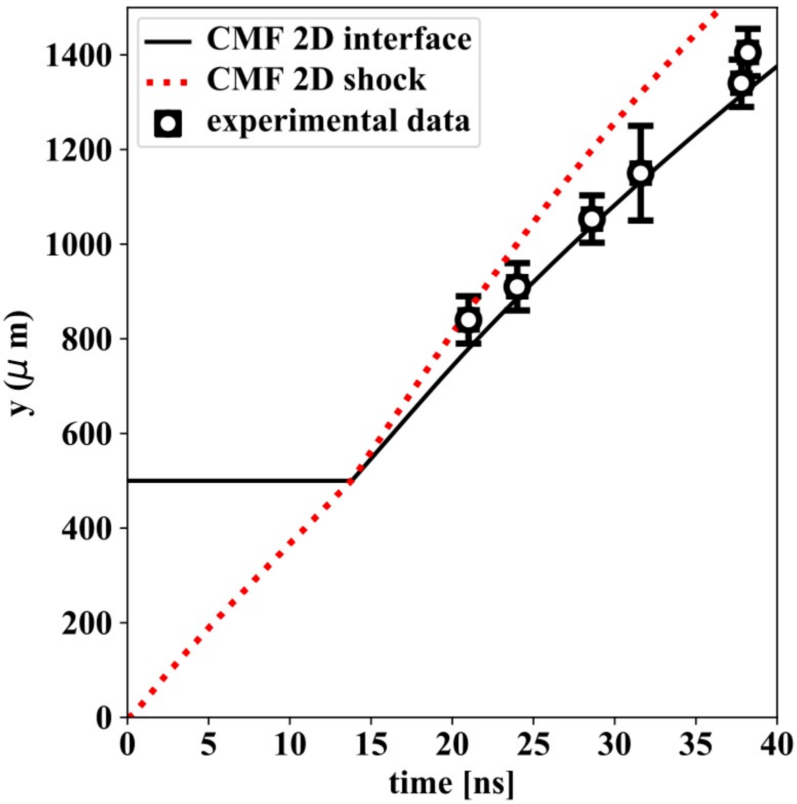


Figure 13. Shock and interface behavior for the 2D version of the previous simulation. This calculation produces a similar but slightly slower shock /interface speed as the 1D version, which is typical for such simulations.

Comparing the plot in Figure 13 to the first frame in the previous figure, we see that the behavior of the two simulations is similar, with the shock and interface motion being slightly slower in 2D. This is expected for a simulation of a quasi-planar experiment, due to the possibility for lateral decompression when the second dimension is introduced as well as a more complete description of any potential scattering losses. These results have all been published in the open literature [Di Stefano19].

Finally, we note that having this experiment in the CMF has facilitated the modeling of a new experiment, that has already been fielded on OMEGA-EP. This new experiment uses a configuration similar to *ModCons*, but modified to produce a system and drive more similar to the NIF experiment *MShock*. Having an established experiment in the CMF streamlined the process of creating the new simulation while ensuring consistent modeling choices.

MShock (OMEGA)

The OMEGA *MShock* experiment is a planar instability experiment, consisting of two opposing plastic ablators with a thick layer of foamed plastic in between them. At some location within the foam, we place another, thinner layer of solid plastic. Each ablator is directly driven, producing two counterpropagating shocks moving towards the thin layer. This allows us to study feed-through effects under reshock, as the layer is sufficiently thin that its two surfaces cannot be considered independent interfaces. An image of the pre-experiment system is shown in Figure 14.

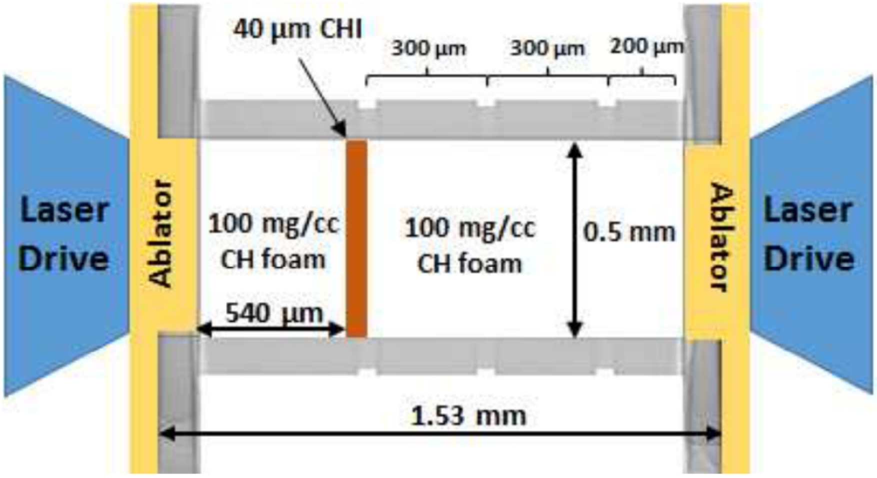


Figure 14. A pre-experiment radiograph of an OMEGA *MShock* target, showing relevant parts of the system. The shocked behavior of the orange layer is the focus of this experiment.

The simulation is not driven by the laser model. Instead, we used three energy sources: two to model the laser drive as initially-thin deposition regions on the outer surfaces of the ablators and a third to model preheat expansion of the thin layer prior to shock arrival. In addition to the energy sources, the simulation requires the hydrodynamics package and the BHR mix model in order to correctly model the experiment. Comparison of the thin-layer growth with and without use of the mix model, as modeled using CMF-generated decks, is shown in Figure 15.

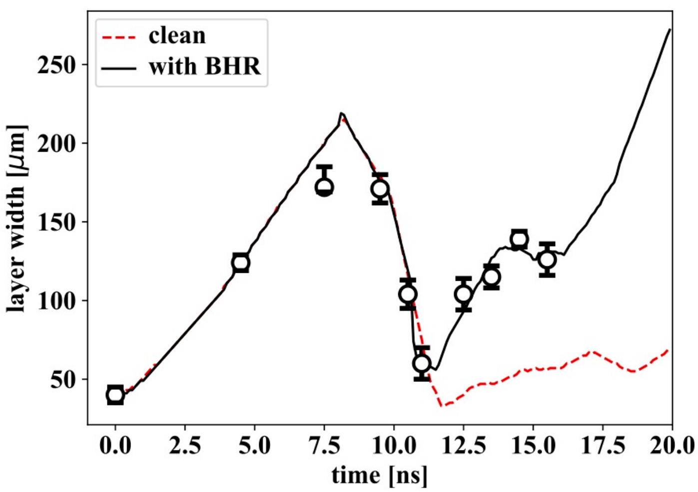


Figure 15. Evolution of the width of the thin layer in the OMEGA *MShock* experiment under preheat, shock, and finally reshock. The solid black and dashed red curves show the simulated result as produced using 1D CMF-generated decks, with and without BHR. Including the mix model allows the simulation to compare favorably with experiment.

In the figure, growth from 0 to about 8 ns is due to preheat, prior to shock arrival. The two shocks transit the thin layer at nearly the same time; the arrival of the first is indicated by the recompression beginning at 8 ns, and the arrival of the second is indicated by the increase in compression rate starting at about 10 ns. The shocks exit the thin layer at around 11 ns, and the remainder of the evolution is due to a combination of mix and shock/rarefaction reverberation in the thin layer. This work has been published [Desjardins19, Desjardins21]; however, the original decks used to produce the computational results in those papers no longer exist and had to be reconstructed. The new version produces growth that is nearly identical to the original, and in fact agrees better with experiment near the latest-time data points.

This result is an excellent demonstration of the ability of the xRAGE code to successfully model the effects of three complex physical processes in quick succession: preheat, shock compression, and hydrodynamic mix. Without the mix model, the code can reproduce the experiment well through the first two phases, but fails to reproduce the third. Using BHR, the code can correctly capture the growth in the third phase both qualitatively and quantitatively.

Cylinders (OMEGA)

The OMEGA and NIF-based *Cylinders* experiment is a cylindrical instability platform. *Cylinders* is a direct-drive platform for studying cylindrical implosions to measure deceleration-phase Rayleigh-Taylor instability (RTI) growth which can significantly affect the inertial confinement fusion implosion's performance. The *Cylinders* platform is well-suited for the measurement of deceleration-phase RTI growth because it allows for direct diagnostic access to the converging interface by imaging down the cylinder, while maintaining convergence effects.

The *Cylinders* platform is three-dimensional (see Figure 16), with a sinusoidal perturbation of the inner surface of the Al marker layer, given by the formula R() = R_o + COS (m), where R_o is the average radius, is the amplitude of the perturbation, and m is the mode of the perturbation.

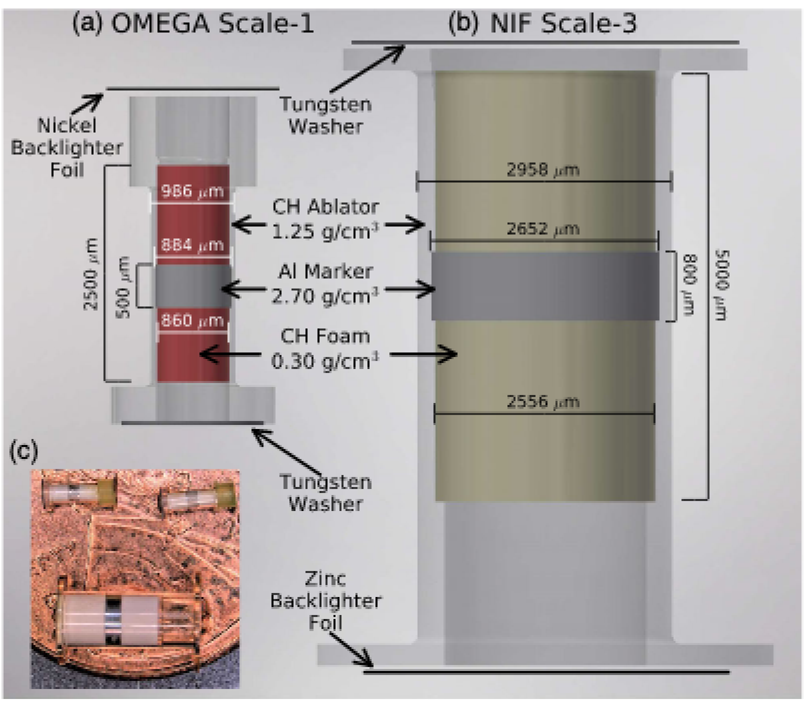


Figure 16. (a) Schematic of the scale-1 cylindrical target fielded at OMEGA, (b) scale-3 target fielded at the NIF, and (c) two OMEGA targets(top) and one NIF target (bottom) on the surface of a penny. (Figure and Caption from Sauppe et al. Phys. Rev. Lett. 124, 185003 (2020). I plan to make an adapted figure for the next version of this milestone document.

To model this inherently three-dimensional platform, two models are used: a cylindrical-axisymmetric model without the perturbation (R-Z) and a planer model of a slice through the perturbation and marker layer (R-) (see Figure 17). The simulations are both driven by the laser model, which requires the heat conduction, isotopics, and 3T packages. Additionally, the simulation requires the hydrodynamics package. While the R- model captures the evolution of the perturbation as the implosion evolves, the R-Z model captures the axial uniformity of the imploding marker layer. The R-Z CMF-generated input deck presently requires the by-hand addition of a dezoning block to run to completion of the experiment. The results presented here include this addition; near-term future work is to add the ability to dezone regions into the CMF and this experiment. Results from CMF-generated input decks for R- and R-Z geometries are captured in Figure 18.

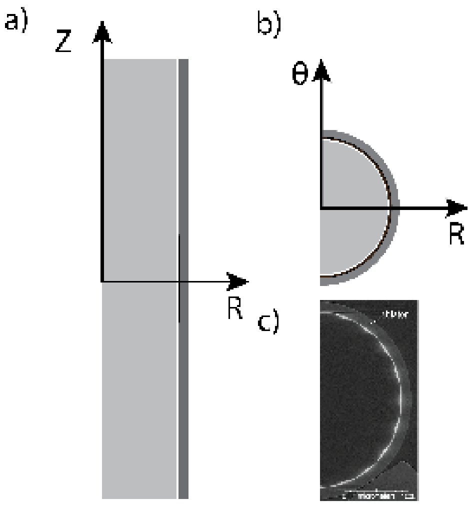


Figure 17. Schematic of simulation setup for the a) axisymmetric R-Z-geometry and b) R--geometry. The Al marker layer is black, the foam fill is the light gray inner layer, and the dark grey outer layer is the plastic ablator. c) CT scan of NIF target with machined initial perturbation on the inner surface of the Al marker.

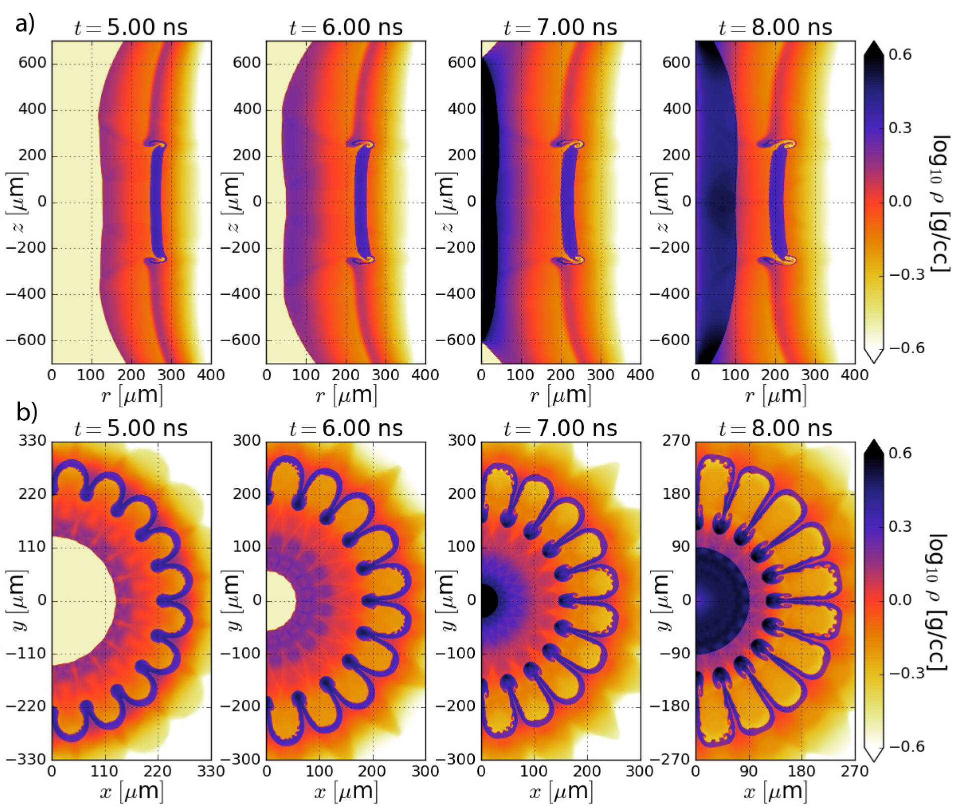


Figure 18. Density snapshots from CMF-generated 2D laser-driven (a) R- and (b) R-Z calculations. Capturing the implosion (5 & 6 ns) and the reflected shock (7 & 8 ns).

In Figure 18, the implosion of the marker layer including the formation of bubbles and spikes is clearly seen. Also the calculations indicate a slight bowing of the marker layer along the axial direction. The trajectory of the outer spike, bubble, inner spike, and shock from the CMF-generated simulations are compared to data from 4 OMEGA shots.

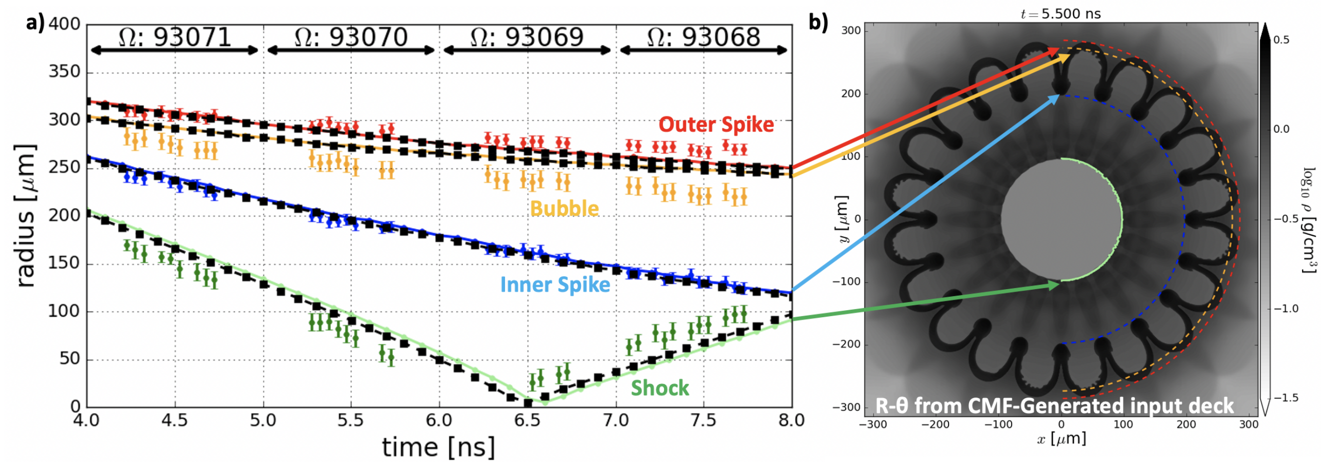


Figure 19. (a) Implosion trajectories extracted from the density output from CMF-generated R- calculations (colors solid) and benchmarked calculations (black dashed); (b) density at 5.5 ns from CMF generated input deck.

This result shows the ability of CMF-generated input decks to nearly match benchmarked input decks and is another excellent demonstration of the ability of the xRAGE code to successfully model the effects of three complex physical processes. The slight differences between the CMF-generated input deck and the benchmarked deck arise from slight differences in the implementation of the laser package and the use of a dezone region in the benchmarked deck. These differences can be eliminated with careful implementation of the laser package and use of a dezone region. The code can reproduce the experiment well through both the implosion and reshock phases.

Summary

In summary, the goal of the milestone was to provide an initial implementation of HED experiments in the CMF through Authority and model development. The HED Hydrodynamics Project has implemented a common methodology for modeling high energy density (HED) experiments by extending development of the EAPA Authority to include relevant physics models, customization tools and templates, and in situ and post-processing capabilities. Several models for small-scale HED experiments were successfully added to the CMF and simulations reproduce the results of preexisting, benchmarked input decks. Additionally, we note that having these experiments in the CMF facilitated the modeling of a new experiment that has already been fielded. Having an established experiment in the CMF streamlined the process of creating the new simulation while ensuring consistent modeling choices.

To review, the final products of the milestone include:

1. CMF implementations of specific features and physics options required to incorporate HED models in the EAPA Authority, including
   a. Expansion of general functionality of the CMF and the EAPA Authority
   b. 1D and 2D laser package options
   c. Heat conduction options
   d. 3T plasma physics options
   e. Mix modeling options

    f. User control of EOS tables
    g. Freeze regions
    h. 1D primitives
2. Implementation of HED models into the CMF
    a. 1D and 2D ModCons with no laser
    b. 1D and 2D ModCons with laser package
    c. 1D and 2D MShock OMEGA models
    d. 2D Cylinders models in cylindrical-axisymmetric R-Z geometry and planar R-Theta geometry
3. Implementation of HED templates to expedite new experiment creation in EAPA
4. Implementation of in situ and post-processing tools for HED experiments, using *RageView* and *Fusion*
5. Customization examples
6. A step-by-step tutorial in Confluence on using the CMF
7. This report available on Confluence and as a white paper documenting the work performed for this milestone

Future work

Future plans include expanding the current physics packages available through the EAPA Authority to incorporate additional options implemented in the codes, as well as support new options. These include:

1. Heat conduction
    a. Implement tabular SESAME conduction (this was previously hardcoded in a way that precluded use of other models and, therefore, was turned off temporarily)
    b. Implement test models, e.g., a simpler Spitzer-like model that assumes full ionization, as well as analytic power-law model
2. Radiation transport: diffusion
3. Turbulence modeling: Local Wave Number Model (LWN)
4. DZN regions
5. Support for 3D models
6. Laser options
    a. Support for specifying rings to permit multiple pulses and/or beam profiles
    b. Support for Cross-beam Energy Transfer (CBET) model
7. Post-processing
    a. Support for *ParaView* in situ adaptor in EAPA when xRAGE version is incremented
    b. Sevelop synthetic radiographs in post-processing

Additionally, we have FY22 plans to improve the machinery that enables Authorities to share physics options.

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